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SOME EXPERIMENTAL RESULTS CONCERNING  
THE ERROR PROPAGATION IN RUNGE-KUTTA  
TYPE INTEGRATION FORMULAS

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16. Abstract  This report deals with the global error propagation of RUNGE-KUTTA formulas. The problem is approached in two different ways. Section I presents the more conventional approach using the integrated differential equation for the error propagation. In Section II, two-sided (or bilateral) RUNGE-KUTTA formulas are derived. Knowledge of the leading term of the local truncation error is essential for both approaches.			
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# SOME EXPERIMENTAL RESULTS CONCERNING THE ERROR PROPAGATION IN RUNGE-KUTTA TYPE INTEGRATION FORMULAS

## INTRODUCTION

1. In two earlier reports [1], [2], the author derived RUNGE-KUTTA formulas up to the eighth order. Each of these formulas, in fact, represented a pair of RUNGE-KUTTA formulas. By adding one or two more evaluations of the differential equation and changing the weight factors, the  $n$ th-order formula ( $n \leq 8$ ) was extended to a  $(n+1)$ st-order formula.
2. In these earlier reports, the  $(n+1)$ st-order formula was used as a step-size control for the  $n$ th-order formula since the  $(n+1)$ st-order formula covers correctly the leading term of the local truncation error of the  $n$ th-order formula.
3. In this report we shall deal with the global error propagation of our RUNGE-KUTTA formulas. The problem will be approached in two different ways. In Section I, we will present the more conventional approach using the integrated differential equation for the error propagation. In Section II, two-sided (or bilateral) RUNGE-KUTTA formulas are derived. Such two-sided RUNGE-KUTTA formulas are convenient for the investigation of the error propagation of extensive systems of differential equations, since no partial derivatives of the differential equations are required for this type of formulas.
4. For both approaches the knowledge of the leading term of the local truncation error is essential. In the first approach, the local truncation error enters directly the equation for the error propagation. For the second approach, our RUNGE-KUTTA formulas can be easily converted into two-sided formulas by making use of the leading term of the local truncation error of our formulas.
5. As described in Section I and Section II, both approaches for the error propagation can serve to obtain realistic upper and lower bounds for the error, along with the integration of the differential equations of the problem. In general, the true error will lie somewhere between these bounds. However, certain conditions have to be satisfied to guarantee

that the true error is always located between these bounds. If such conditions can be formulated, they probably would be of little practical help because they would be too complicated and would involve unknown partial derivatives. This report will not be concerned with the formulation of such conditions. Section III, however, will present some nontrivial examples to show that our procedures are capable of yielding reasonably close error bounds for the solutions of such problems.

## SECTION I. THE ERROR EQUATIONS, BASED ON ONE INTEGRATION PROCEDURE PER INTEGRATION STEP

6. For simplicity, let us consider a system of only two first-order differential equations:

$$\left. \begin{aligned} \frac{dx}{dt} &= f(t, x, y) \\ \frac{dy}{dt} &= g(t, x, y) \end{aligned} \right\} \quad (1)$$

The numerical integration of (1) is performed by a RUNGE-KUTTA formula. For the first equation (1), such a RUNGE-KUTTA formula would read

$$\left. \begin{aligned} f_0 &= f(t_0, x_0, y_0) \\ f_1 &= f(t_0 + \alpha_1 h, x_0 + h\beta_{10}f_0, y_0 + h\beta_{10}g_0) \\ f_2 &= f[t_0 + \alpha_2 h, x_0 + h(\beta_{20}f_0 + \beta_{21}f_1), y_0 + h(\beta_{20}g_0 + \beta_{21}g_1)] \\ &\vdots \\ &\vdots \\ &\vdots \end{aligned} \right\} \quad (2)$$

and

$$x = x_0 + h(c_0f_0 + c_1f_1 + c_2f_2 + \dots) \quad (3)$$

The coefficients  $\alpha_1, \alpha_2, \dots$ ;  $\beta_{10}, \beta_{20}, \beta_{21}, \dots$ ; and  $c_0, c_1, c_2, \dots$  are known numerical constants of the RUNGE-KUTTA formula, and  $h(= dt)$  stands for the integration stepsize.



A corresponding RUNGE-KUTTA formula holds for the second differential equation (1).

7. We now assume that the values  $x_0$  and  $y_0$  at the beginning  $t = t_0$  of our integration step are affected by errors  $(\epsilon_x)_0$  and  $(\epsilon_y)_0^1$ , and we like to study the propagation of these errors through the current integration step.

Including these errors in (2) and (3), we obtain

$$\left. \begin{aligned} \tilde{f}_0 &= f[t_0, x_0 + (\epsilon_x)_0, y_0 + (\epsilon_y)_0] \\ \tilde{f}_1 &= f[t_0 + \alpha_1 h, x_0 + (\epsilon_x)_0 + \beta_{10} \tilde{f}_0 h, y_0 + (\epsilon_y)_0 + \beta_{10} \tilde{g}_0 h] \\ \tilde{f}_2 &= f[t_0 + \alpha_2 h, x_0 + (\epsilon_x)_0 + (\beta_{20} \tilde{f}_0 + \beta_{21} \tilde{f}_1)h, \\ &\quad y_0 + (\epsilon_y)_0 + (\beta_{20} \tilde{g}_0 + \beta_{21} \tilde{g}_1)h] \\ &\vdots \\ &\vdots \\ &\vdots \end{aligned} \right\} \quad (4)$$

$$x + \epsilon_x = x_0 + (\epsilon_x)_0 + h(c_0 \tilde{f}_0 + c_1 \tilde{f}_1 + c_2 \tilde{f}_2 + \dots) \quad (5)$$

If we expand (4) in TAYLOR series and carry only linear terms in  $(\epsilon_x)_0$  and  $(\epsilon_y)_0$ , the following expressions result:

- 
1. We disregard errors in  $t_0$  since such errors can be avoided by a proper selection of the time step. For a binary electronic computer, time steps that are a (positive or negative) power of 2 should be used.

$$\left. \begin{aligned}
\tilde{f}_0 &= f_0 + \left( \frac{\partial f}{\partial x} \right)_{000} (\epsilon_x)_0 + \left( \frac{\partial f}{\partial y} \right)_{000} (\epsilon_y)_0 \\
\tilde{f}_1 &= f_1 + \left( \frac{\partial f}{\partial x} \right)_{100} \left[ (\epsilon_x)_0 + \beta_{10} (\tilde{f}_0 - f_0) h \right] \\
&\quad + \left( \frac{\partial f}{\partial y} \right)_{100} \left[ (\epsilon_y)_0 + \beta_{10} (\tilde{g}_0 - g_0) h \right] \\
\tilde{f}_2 &= f_2 + \left( \frac{\partial f}{\partial x} \right)_{200} \left\{ (\epsilon_x)_0 + \left[ \beta_{20} (\tilde{f}_0 - f_0) + \beta_{21} (\tilde{f}_1 - f_1) \right] h \right\} \\
&\quad + \left( \frac{\partial f}{\partial y} \right)_{200} \left\{ (\epsilon_y)_0 + \left[ \beta_{20} (\tilde{g}_0 - g_0) + \beta_{21} (\tilde{g}_1 - g_1) \right] h \right\}
\end{aligned} \right\} \quad (6)$$

The three subscripts  $\nu 00 (\nu = 0, 1, 2, \dots)$  in (6) are supposed to indicate that the expression in question is to be taken at  $t_0 + \alpha_\nu h$ ,  $x_0, y_0$  ( $\alpha_0 = 0$ ). For example  $\left( \frac{\partial f}{\partial x} \right)_{200}$  stands for  $\left( \frac{\partial f}{\partial x} \right)$  taken at  $t_0 + \alpha_2 h$ ;  $x_0, y_0$ . Introducing (6) into (5) yields an expression for the error  $\epsilon_x$  at the end of the integration step. If, in this expression, we restrict ourselves to linear terms in  $h$ , we may drop in (6) all terms that are multiplied with  $h$  and may replace  $\left( \frac{\partial f}{\partial x} \right)_{\nu 00}$  by  $\left( \frac{\partial f}{\partial x} \right)_{000}$  and  $\left( \frac{\partial f}{\partial y} \right)_{\nu 00}$  by  $\left( \frac{\partial f}{\partial y} \right)_{000}$  since

$$\left. \begin{aligned}
\left( \frac{\partial f}{\partial x} \right)_{\nu 00} &= \left( \frac{\partial f}{\partial x} \right)_{000} + \left( \frac{\partial^2 f}{\partial x \partial t} \right)_{000} \alpha_\nu h + \dots \\
\left( \frac{\partial f}{\partial y} \right)_{\nu 00} &= \left( \frac{\partial f}{\partial y} \right)_{000} + \left( \frac{\partial^2 f}{\partial y \partial t} \right)_{000} \alpha_\nu h + \dots
\end{aligned} \right\} \quad (7)$$

Because of the equation of condition

$$c_0 + c_1 + c_2 + \dots = 1 \quad (8)$$

for the RUNGE-KUTTA coefficients, the expression for  $\epsilon_x$  and the corresponding expression for  $\epsilon_y$  then read

$$\left. \begin{aligned} \epsilon_x &= (\epsilon_x)_0 + \left[ \left( \frac{\partial f}{\partial x} \right)_0 (\epsilon_x)_0 + \left( \frac{\partial f}{\partial y} \right)_0 (\epsilon_y)_0 \right] \cdot h \\ \epsilon_y &= (\epsilon_y)_0 + \left[ \left( \frac{\partial g}{\partial x} \right)_0 (\epsilon_x)_0 + \left( \frac{\partial g}{\partial y} \right)_0 (\epsilon_y)_0 \right] \cdot h \end{aligned} \right\} \quad (9)$$

In (9), we have replaced the triple subscript 000 of the partial derivatives by just one subscript 0.

Equation (9) represents the propagation of the error  $(\epsilon_x)_0, (\epsilon_y)_0$  through the current integration step. To obtain the total error, we still have to add to the right-hand sides of (9) the local truncation and local round-off error committed during the current integration step.

Denoting these errors by  $T_x, T_y$  and  $R_x, R_y$ , respectively, we obtain instead of (9) in vector form

$$\begin{pmatrix} \epsilon_x \\ \epsilon_y \end{pmatrix} = \begin{pmatrix} \epsilon_x \\ \epsilon_y \end{pmatrix}_0 + \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} \end{pmatrix}_0 \begin{pmatrix} \epsilon_x \\ \epsilon_y \end{pmatrix}_0 \cdot h + \begin{pmatrix} T_x \\ T_y \end{pmatrix} + \begin{pmatrix} R_x \\ R_y \end{pmatrix} \quad (10)$$

In an obvious way, equation (10) can be extended to systems of more than two first-order differential equations.

8. To handle these well-known equations (10) for the error propagation, the partial derivatives  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial g}{\partial x}, \frac{\partial g}{\partial y}$  have to be computed along with the integration of the differential equations. Furthermore, certain assumptions have to be made for the local truncation errors  $T_x, T_y$

and the local round-off errors  $R_x, R_y$ . In the following, such assumptions for these errors will be discussed.

9. As for the truncation error, we restrict ourselves to the leading term of this error. In our earlier reports [1],[2], we already determined the leading truncation error term for RUNGE-KUTTA formulas up to the eighth order. This leading term of the local truncation error was used in these earlier reports for the stepsize control only. We introduce this term now also in (10) for  $T_x$  and  $T_y$ .
10. An accurate determination of the round-off errors  $R_x$  and  $R_y$  in (10) is almost impossible. We therefore resort to a somewhat crude but easily obtainable approximation. In (3), the quantities  $x_0$  and  $h(c_0f_0 + c_1f_1 + c_2f_2 + \dots)$  are in general of different order of magnitude, the latter expression being a small increment of  $x_0$ . Therefore, when performing their addition in (3), the electronic computer has to shift a certain part of the smaller number  $h(c_0f_0 + c_1f_1 + c_2f_2 + \dots)$  out of its range. The shifted-out part of the smaller number is lost for the computation. We now consider this shifted-out part as an approximation for the round-off error  $R_x$  in (10). Naturally, the functions  $f_0, f_1, f_2, \dots$  in (2) are also affected by round-off errors. However, when these functions enter equation (3), their round-off errors are multiplied by the small quantity  $h$  and may therefore be neglected, compared with the round-off error resulting from the addition of  $x_0$  and  $h(c_0f_0 + c_1f_1 + c_2f_2 + \dots)$ .

In the same way, an approximate value for the round-off error  $R_y$  can be obtained from the formula for  $y$  that corresponds to (3).

11. Introducing the approximate values  $T_x, T_y$  and  $R_x, R_y$ , the partial derivatives  $\left(\frac{\partial f}{\partial x}\right)_0, \left(\frac{\partial f}{\partial y}\right)_0, \left(\frac{\partial g}{\partial x}\right)_0, \left(\frac{\partial g}{\partial y}\right)_0$  and the total errors  $(\epsilon_x)_0, (\epsilon_y)_0$  at the beginning of the current integration step into the equations (10), the total errors  $\epsilon_x, \epsilon_y$  at the end of the current integration step are easily obtained by a few multiplications and additions.

We evaluated equations (10) three times:

$$\begin{pmatrix} \epsilon_x^{(\nu)} \\ \epsilon_y^{(\nu)} \end{pmatrix} = \begin{pmatrix} \epsilon_x^{(\nu)} \\ \epsilon_y^{(\nu)} \end{pmatrix} + \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} \end{pmatrix}_0 \begin{pmatrix} \epsilon_x^{(\nu)} \\ \epsilon_y^{(\nu)} \end{pmatrix}_0 \cdot h + \begin{pmatrix} T_x \\ T_y \end{pmatrix} + \begin{pmatrix} \nu \cdot R_x \\ \nu \cdot R_y \end{pmatrix} \quad (11)$$

( $\nu = 0, 1, 2$ ).

For  $\nu = 1$  we took proper care of the round-off errors  $R_x, R_y$ , thereby obtaining approximations  $\epsilon_x^{(1)}, \epsilon_y^{(1)}$  for the true errors. For  $\nu = 0$  (disregarding the round-off errors) and for  $\nu = 2$  (doubling the round-off errors) we established "bounds"  $\epsilon_x^{(0)}, \epsilon_y^{(0)}$  and  $\epsilon_x^{(2)}, \epsilon_y^{(2)}$  for the true errors.

Compensating for these errors  $\epsilon_x^{(\nu)}, \epsilon_y^{(\nu)}$ , we obtained from  $x, y$  for  $\nu = 1$  approximations  $x^{(1)}, y^{(1)}$  for the true values  $x_T, y_T$ . For  $\nu = 0$  and  $\nu = 2$ , the compensation yields bounds  $x^{(0)}, y^{(0)}$  and  $x^{(2)}, y^{(2)}$  for  $x_T$  and  $y_T$ . The values  $x, y$  were the results of the RUNGE-KUTTA integration (2), (3) of our problem without any error compensation.

Figure 1 illustrates the procedure for the computation of the error spread in  $x$  for the first two integration steps.

12. As already stated in the Introduction, we cannot always expect strict bounds using such an extremely simplified approximation procedure for the round-off errors. However, the examples of Section III show that by using in (11) the correct values of the partial derivatives and proper approximations for the local truncation errors, realistic and reasonably close error bounds are obtainable by our procedure for the round-off errors.

In some problems, it might occur that our "bounds" are too tight. In such cases, the values  $x^{(0)}$ ,  $x^{(1)}$ , and  $x^{(2)}$  (or the corresponding values of  $y$ ) would become practically equal, but not necessarily equal to the true value,  $x_T$ . Better bounds might then be obtained by replacing in (11)  $\nu = 0, 1, 2$  by  $\nu = -1, 1, 3$  or similar values to effect a wider spread of the bounds.

13. If the partial derivatives in (10) assume large values during the numerical integration of the problem (1), the error can propagate heavily, even if the local truncation errors  $T_x$  and  $T_y$  are kept very small by a sufficiently small integration stepsize. To slow down such an undesirably large error spread, we introduce an additional test for the stepsize by

requiring that the products  $\left| \left( \frac{\partial f}{\partial x} \right)_0 \right| h$ ,  $\left| \left( \frac{\partial f}{\partial y} \right)_0 \right| h$ ,  $\left| \left( \frac{\partial g}{\partial x} \right)_0 \right| h$  and

$\left| \left( \frac{\partial g}{\partial y} \right)_0 \right| h$  should not exceed a pre-given value. If they exceed that value, the stepsize  $h$  will be halved sufficiently often until all products stay below the pre-given value.

By a proper choice of this pre-given test value, we can regulate the error spread to a certain extent. However, one should keep in mind that a very small test value might lead to very small integration stepsizes. Thereby, a heavy buildup of the round-off errors might occur, resulting in unrealistically large error bounds.

## SECTION II. THE ERROR EQUATIONS, BASED ON TWO INTEGRATION PROCEDURES PER INTEGRATION STEP

14. Although the method of Section I, if properly applied, will lead to rather accurate values for the errors and reasonably close error bounds, the method has the disadvantage of requiring the computation of the partial

derivatives  $\left( \frac{\partial f}{\partial x} \right)_0$ ,  $\left( \frac{\partial f}{\partial y} \right)_0$ ,  $\dots$ . These partial derivatives might turn out to be lengthy and cumbersome expressions. Furthermore, for extensive systems of differential equations there will be a large number of such partial derivatives ( $n^2$  partial derivatives for a system of  $n$  differential equations).

15. To avoid these inconveniences in the study of the error propagation, one might rather resort to methods which do not involve partial derivatives. Such methods can be established if for each step the numerical integration is performed twice by means of two different RUNGE-KUTTA formulas. These two RUNGE-KUTTA formulas are chosen in such a way that their leading terms of the local truncation error are equal but of opposite sign.

Obviously, the arithmetic mean of these two RUNGE-KUTTA formulas represents a RUNGE-KUTTA formula of order  $n+1$ , if the two original RUNGE-KUTTA formulas are of order  $n$ . Considering this arithmetic mean formula as an approximation of the true values, the difference in the values of the original two formulas can be regarded as an indicator for the spread of the truncation error.

In the literature, two such RUNGE-KUTTA formulas are called two-sided or bilateral RUNGE-KUTTA formulas.

Since such two-sided RUNGE-KUTTA formulas do not consider the round-off errors, these must be kept negligible. This means, the error propagation obtained from two-sided RUNGE-KUTTA formulas will be reliable only as long as the truncation errors are dominant compared with the round-off errors.

Because of the dominance of the truncation errors, the error bounds of two-sided RUNGE-KUTTA formulas will not be as close as the bounds of the procedure described in Section I. This is not surprising, since the truncation errors can be practically eliminated in the procedure of Section I.

16. Two-sided RUNGE-KUTTA formulas of low order have been known a long time. For example, the modified EULER-CAUCHY formula

$$x = x_0 + \frac{1}{2} h \{f(t_0, x_0) + f[t_0 + h, x_0 + hf(t_0, x_0)]\} \quad , \quad (12)$$

which represents a RUNGE-KUTTA formula of the second order, can be considered as the arithmetic mean of the two first-order RUNGE-KUTTA formulas:

$$\left. \begin{aligned} x^{(1)} &= x_0 + hf(t_0, x_0) \\ x^{(2)} &= x_0 + hf[t_0 + h, x_0 + hf(t_0, x_0)] \end{aligned} \right\} \quad (13)$$

TAYLOR-expansion of the right-hand sides of (13) leads to:

$$\left. \begin{aligned} x^{(1)} &= \left[ x_0 + hf(t_0, x_0) + \frac{1}{2} h^2 (f_t + f_x f)_0 \right] \\ &\quad - \frac{1}{2} h^2 (f_t + f_x f)_0 + \dots \\ x^{(2)} &= \left[ x_0 + hf(t_0, x_0) + \frac{1}{2} h^2 (f_t + f_x f)_0 \right] \\ &\quad + \frac{1}{2} h^2 (f_t + f_x f)_0 + \dots \end{aligned} \right\} \quad (14)$$

Since the last terms on the right-hand sides of (14) represent the leading terms of the local truncation error of formulas (13), these formulas are indeed two-sided RUNGE-KUTTA formulas of the first order.

In the case of formulas (12) and (13), the conditions that (13) always yields strict bounds for the solution (12) have been established by S. GORN and R. MOORE [3]. These conditions are also quoted in another paper by S. GORN ([4], p. 76). They involve the first- and second-order partial derivatives  $f_t$ ,  $f_{tt}$ ,  $f_{tx}$  and  $f_{xx}$ .

More recently, two-sided RUNGE-KUTTA formulas of the second- and third-order were published by A.D. GORBUNOV and YU. A. SHAKHOV [5], [6].

17. Two-sided RUNGE-KUTTA formulas, up to the eighth order, can be obtained easily from the RUNGE-KUTTA formulas of our reports [1], [2]. We have only to recall that the formulas of these reports represent pairs of RUNGE-KUTTA formulas of the order  $n$  and  $n+1$  ( $1 \leq n \leq 8$ ). The formula of the order  $n+1$  is obtained from the formula of the order  $n$  by adding one or two more evaluations of the differential equations and changing the weight factors  $c_k$  of the  $n$ th-order formula to the weight factors  $\hat{c}_k$  of the  $(n+1)$ st-order formula.



Knowing two such formulas of the  $n$ th- and the  $(n+1)$ st-order, one can immediately derive from these formulas two two-sided RUNGE-KUTTA formulas of the  $n$ th-order by putting

$$\left. \begin{aligned} c_K^{(1)} &= 2\hat{c}_K - c_K \\ c_K^{(2)} &= c_K \end{aligned} \right\} \quad (15)$$

However, it is not even necessary to compute the coefficients (15), since we can operate our RUNGE-KUTTA formulas of [1],[2] as two-sided RUNGE-KUTTA formulas in the following way: Starting from the initial values  $(t_0, x_0^{(1)}, \dots)$ , we compute one step by our  $n$ th-order RUNGE-KUTTA formula applying the leading term TE of the local truncation error for the stepsize control. From the result, we subtract twice the term TE, thereby obtaining the values  $x^{(1)}, \dots$  for one of our two-sided RUNGE-KUTTA formulas. Next, we start from the initial values  $(t_0, x_0^{(2)}, \dots)$  and compute one step with the same stepsize as for  $x^{(1)}$ , thereby obtaining the values  $x^{(2)}$  for our second two-sided RUNGE-KUTTA formula.

In Figure 2 the procedure is illustrated for the first two integration steps. The final values  $x$  are then approximated by

$$x = \frac{1}{2} [x^{(1)} + x^{(2)}] , \quad (16)$$

and the propagated errors by

$$\epsilon_x = \frac{1}{2} [x^{(1)} - x^{(2)}] \quad (17)$$

Corresponding formulas hold for  $y$ ,  $\epsilon_y$  and for any further dependent variables.

18. For the convenience of the reader, we have listed as Appendix to this report our RUNGE-KUTTA coefficients for RK1(2), RK2(3),  $\dots$ , RK7(8) from [2],[1], including the leading term TE of the local

truncation error. However, formulas RK1(2) and RK2(3) in [2] have been changed to formulas more suitable for the study of error propagation. For the somewhat lengthy table of coefficients for RK8(9) we refer to our paper [1].

19. While the local truncation error can be checked by the term TE of the Appendix, we have control of the error propagation during the current integration step by checking  $|\epsilon_x - (\epsilon_x)_0|$ ,  $|\epsilon_y - (\epsilon_y)_0|$ , etc., since these expressions represent the error growth during the current integration step (the suffix 0 indicating the values at the beginning of the current step). By requiring that the expressions  $|\epsilon_x - (\epsilon_x)_0|$ ,  $|\epsilon_y - (\epsilon_y)_0|$ , etc. remain smaller than a pre-given small quantity and by reducing the stepsize  $h$  until these condition are met, we have, similar as in the procedure of Section I, a certain control of the error propagation.
20. To get the error propagation of two-sided RUNGE-KUTTA formulas properly started, the local truncation error has to be dominant from the beginning of the integration. Therefore, in the beginning, we relax the tolerance for the leading term of the local truncation error. After the propagated error has grown to a certain magnitude, we continue the computation by using a sharper (smaller) tolerance. In this way, for the examples of Section III, we could keep the error bounds of our two-sided RUNGE-KUTTA formulas relatively close (about three to four times as large as the bounds for the procedure of Section I).

### SECTION III. EXAMPLES FOR THE ERROR PROPAGATION

21. We apply the methods of Sections I and II to the following examples:

Problem I:

$$\left. \begin{aligned} \frac{dx}{dt} &= \frac{1}{2} \cdot \frac{x}{t+1} - 2t \cdot y \\ \frac{dy}{dt} &= \frac{1}{2} \cdot \frac{y}{t+1} + 2t \cdot x \end{aligned} \right\} \quad (18)$$

For the initial values

$$t_0 = 0, \quad x_0 = 1, \quad y_0 = 0, \quad (19)$$

the differential equations (18) have the following solution in closed form:

$$\left. \begin{aligned} x_T &= \sqrt{t+1} \cdot \cos(t^2) \\ y_T &= \sqrt{t+1} \cdot \sin(t^2) \end{aligned} \right\} \quad (20)$$

Figures 3 and 4 show the shape of the (true) solution (20). Because of the argument  $t^2$  in (20), the frequency of the oscillations increases rapidly with  $t$ . The problem clearly requires a continuous stepsize control as provided by our RUNGE-KUTTA formulas. We integrated problem (18), (19) from  $t = 0$  to  $t = 5$ .

Problem II — Restricted Problem of Three Bodies; (see V. SZEBEHELY [7] or other textbooks of celestial mechanics):

In the rotating coordinate system, the problem leads to the well-known differential equations:

$$\left. \begin{aligned} \frac{d^2 x}{dt^2} &= x + 2 \cdot \frac{dy}{dt} - \mu' \cdot \frac{x + \mu}{[(x + \mu)^2 + y^2]^{3/2}} \\ &\quad - \mu \cdot \frac{x - \mu'}{[(x - \mu')^2 + y^2]^{3/2}} \\ \frac{d^2 y}{dt^2} &= y - 2 \cdot \frac{dx}{dt} - \mu' \cdot \frac{y}{[(x + \mu)^2 + y^2]^{3/2}} \\ &\quad - \mu \cdot \frac{y}{[(x - \mu')^2 + y^2]^{3/2}} \end{aligned} \right\} \quad (21)$$

Here,  $x$  and  $y$  represent the coordinates of a moving particle of negligible weight (spaceship) with respect to the barycentric system of the two fixed bodies (earth, moon). In this system, the earth has the constant coordinates  $x_E = -\mu$ ,  $y_E = 0$ , and the moon has the constant coordinates  $x_M = \mu' = 1 - \mu$ ,  $y_M = 0$ .

We solved problem (21) for two different sets of initial values:

$$\text{a. } t_0 = 0, \quad x_0 = 1.15, \quad y_0 = 0, \quad \dot{x}_0 = 0, \quad \dot{y}_0 = -0.87 \left( \mu = \frac{1}{80} \right) \quad (22)$$

and

$$\text{b. } t_0 = 0, \quad x_0 = 1.2, \quad y_0 = 0, \quad \dot{x}_0 = 0, \quad \dot{y}_0 = -0.7 \left( \mu = \frac{1}{80} \right) \quad (23)$$

Figures 10 and 15 show the shape of the orbit for the initial conditions (22) or (23), respectively. The marks along the orbit represent the time scale. The first orbit was computed from  $t = 0$  to  $t = 6$ , the second orbit from  $t = 0$  to  $t = 25$ .

Since no solution in closed form for problem (21), (22) or problem (21), (23) is known, we substituted for the true solution an orbit obtained by carrying more than 20 decimal digits on the computer.<sup>2</sup> The numerical solution of our problems was obtained by carrying 16 digits (IBM-7094).

Since, for some parts of its orbit, the spaceship approaches earth or moon relatively closely but for other parts is carried far away from these bodies, we again need a continuous stepsize control to take proper care of all parts of the orbit.

22. Figures 5 through 9, 11 through 14, and 16 and 17 show our results for the propagated errors  $\Delta x$  of Problems I, IIa, and IIb. The errors  $\Delta y$  look similar, especially in Problem I, and were therefore omitted.

---

2. This part of the computations was carried out by Mr. F. R. Calhoun from the Computer Sciences Corporation (CSC) who also developed the necessary 30- and 40-digit packages for the IBM-7094 computer.

On these graphs we used a few abbreviated expressions that should be explained now:

- a. TOL stands for tolerance. The products  $\text{TOL} \cdot |x_0|$ ,  $\text{TOL} \cdot |y_0|$ , etc. were used as tolerances for the local truncation errors ( $x_0, y_0, \dots$  being the initial values in  $x, y, \dots$  for the current step). The integration stepsize  $h(=dt)$  was selected in such a manner that the local truncation errors  $|TE_x|$ ,  $|TE_y|$ , etc. would not exceed the above products.
- b. TMPDDT stands for test value for the (absolute) maximum of the partial derivatives times  $dt$ . This test value serves as a control for the error propagation; (see No. 13).
- c. TEXY stands for test value for the (accumulated) error in  $x$  or  $y$ . As soon as both of these errors in absolute value exceed TEXY, we switched over from a relaxed tolerance ( $\text{TOL} = 0.1 \cdot 10^{-12}$ ) to a sharper tolerance ( $\text{TOL} = 0.1 \cdot 10^{-16}$ ).
- d. TOLEP stands for tolerance in error propagation. As soon as the maximum of  $|\epsilon_x - (\epsilon_x)_0|$ ,  $|\epsilon_y - (\epsilon_y)_0|$ , etc. exceeds the test value TOLEP, the stepsize  $h(=dt)$  is halved (if necessary repeatedly halved) to prevent a too fast increase in error propagation; (see No. 19).

In all three problems, we printed our results in equidistant time intervals.

In Problems I and IIa we printed for  $\Delta t = \frac{1}{8}$ , in Problem IIb for  $\Delta t = \frac{1}{2}$ . To obtain results for such equidistant time intervals, we had to adjust our stepsize  $h(=dt)$  when overshooting the time interval. In the graphs, the results for the printed time intervals were connected by straight lines.

23. For Problem I, the numerical integration was performed by our RUNGE-KUTTA formulas RK5(6) and RK7(8).

Figures 5, 6, and 7 show the results based on the error propagation formulas of Section I (one integration procedure per integration step).

The curves  $\nu = 0, 2$  or  $\nu = -1, 3$  represent the deviations  $x^{(\nu)} - x^{(1)}$ , where  $x^{(1)}$  stands for the  $x$ -value corrected for the local truncation and round-off error; (see No. 11 and No. 12). The third curve on these graphs, which is mostly close to the  $t$ -axis represents the deviation  $x_T - x^{(1)}$  between the true solution and  $x^{(1)}$ . Naturally, this deviation would be zero if the equations for the error propagation would give results which are completely correct.

We see from Figure 5 that for RK5(6) the error bounds increase from 0 to  $4000 \cdot 10^{-16} = 0.4 \cdot 10^{-12}$ . This means that the 13th place behind the decimal point could be wrong by up to four units. The real error, represented by the third curve in Figure 5, is somewhat smaller than our bounds, namely of the order  $100 \cdot 10^{-16} = 0.01 \cdot 10^{-12}$ . We obtain safe error bounds in this case. Figure 6 shows the error behavior for RK7(8). Here the error bounds are smaller, since the integration is performed in considerably fewer steps. The error bounds do not exceed  $600 \cdot 10^{-16} = 0.6 \cdot 10^{-13}$ . However, because of the larger permissible stepsize, the curve  $x_T - x^{(1)}$  deviates more from zero than in Figure 5. It almost reaches the peaks of the error bound curves.

We recomputed the error behavior for RK7(8) using for the error bounds  $\nu = -1$  and  $\nu = 3$ . The results are plotted in Figure 7. Now the curve  $x_T - x^{(1)}$  fits better between the error bounds which now increase up to  $1200 \cdot 10^{-16} = 0.12 \cdot 10^{-12}$ . Again, we obtain safe error bounds in this case.

Figures 8 and 9 show our results based on the error propagation formulas of Section II (two integration procedures per integration step). The curves represent  $x^{(1)} - x$  and  $x^{(2)} - x$  with  $x = \frac{1}{2} [x^{(1)} + x^{(2)}]$  and as third curve, close to the  $t$ -axis,  $x_T - x$ . The error bounds grow up to  $20\,000 \cdot 10^{-16} = 0.2 \cdot 10^{-11}$  for our formula RK5(6) and up to  $6000 \cdot 10^{-16} = 0.6 \cdot 10^{-12}$  for our formula RK7(8). The actual errors  $x_T - x$  are smaller than these error bounds, so that our bounds, again, can be considered as safe.

Comparing Figures 5, 6, and 7 with Figures 8 and 9, it is very evident that the method of Section I leads, as expected, to closer error bounds than the method of Section II. All Figures show that our error bounds oscillate with approximately the same frequency as the solution itself (Fig. 3).

24. The numerical integration for the orbit of Problem IIa, again, was performed by our RUNGE-KUTTA formulas RK5(6) and RK7(8). Figures 11 to 14 show our results for the error propagation. After the explanations of No. 23, our results need hardly any further interpretation. It is remarkable how the error bounds grow when the spaceship comes close to the earth ( $t \approx 1.5$  and  $t \approx 4.875$ ). Again, our formulas lead to safe error bounds, with larger bounds for RK5(6) than for RK7(8), and the error bounds for the method of Section I are closer than those for the method of Section II.
25. Finally, we integrated Problem IIb by our RUNGE-KUTTA formula RK7(8). Because of the longer time range to be covered in this problem and because of the more complicated shape of the orbit — the spaceship approaches the earth five times — our lower-order formula RK5(6) proved not to be very suitable for this problem. Figures 16 and 17 show the results for our formula RK7(8). Especially in Figure 17, we can easily recognize the increase in the error bounds when the spaceship approaches the earth ( $t \approx 2$ ,  $t \approx 6.5$ ,  $t \approx 12.5$ ,  $t \approx 17.5$ , and  $t \approx 22.5$ ).
26. Although there is no guarantee that the methods of Sections I and II yield strict bounds that bracket the correct solution, we obtained reasonable bounds for the problems of this Section. The bounds bracket the correct solution almost everywhere, and they are also reasonably close to the correct solution. It might require some experience to find the proper values for the test functions involved (TMPDDT or TEXY, TOLEP), especially in problems (such as our Problems IIa and IIb) in which the differential equations contain singularities. In general, it will be advisable to use high-order RUNGE-KUTTA formulas, since their application will keep the propagated errors small. Because such high-order formulas require a relatively small number of integration steps, the errors have no real chance to propagate heavily.

George C. Marshall Space Flight Center

National Aeronautics and Space Administration

Marshall Space Flight Center, Alabama 35812, May 26, 1970

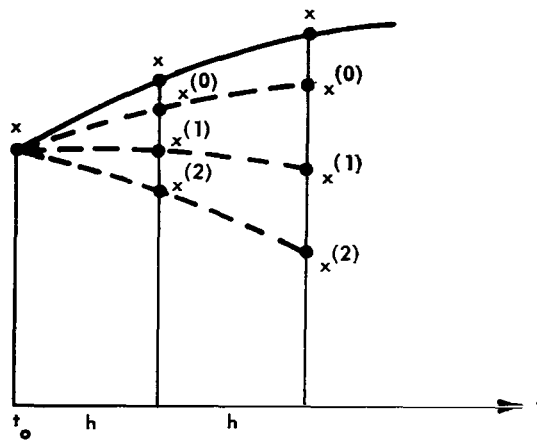


Figure 1. Error spread for methods using one integration procedure per integration step.

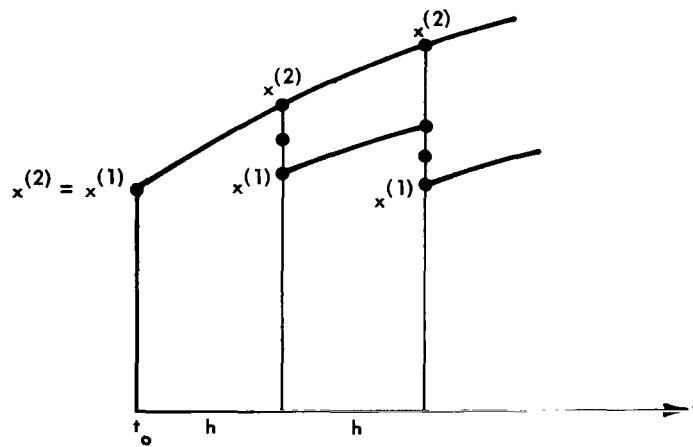


Figure 2. Error spread for methods using two integration procedures per integration step.



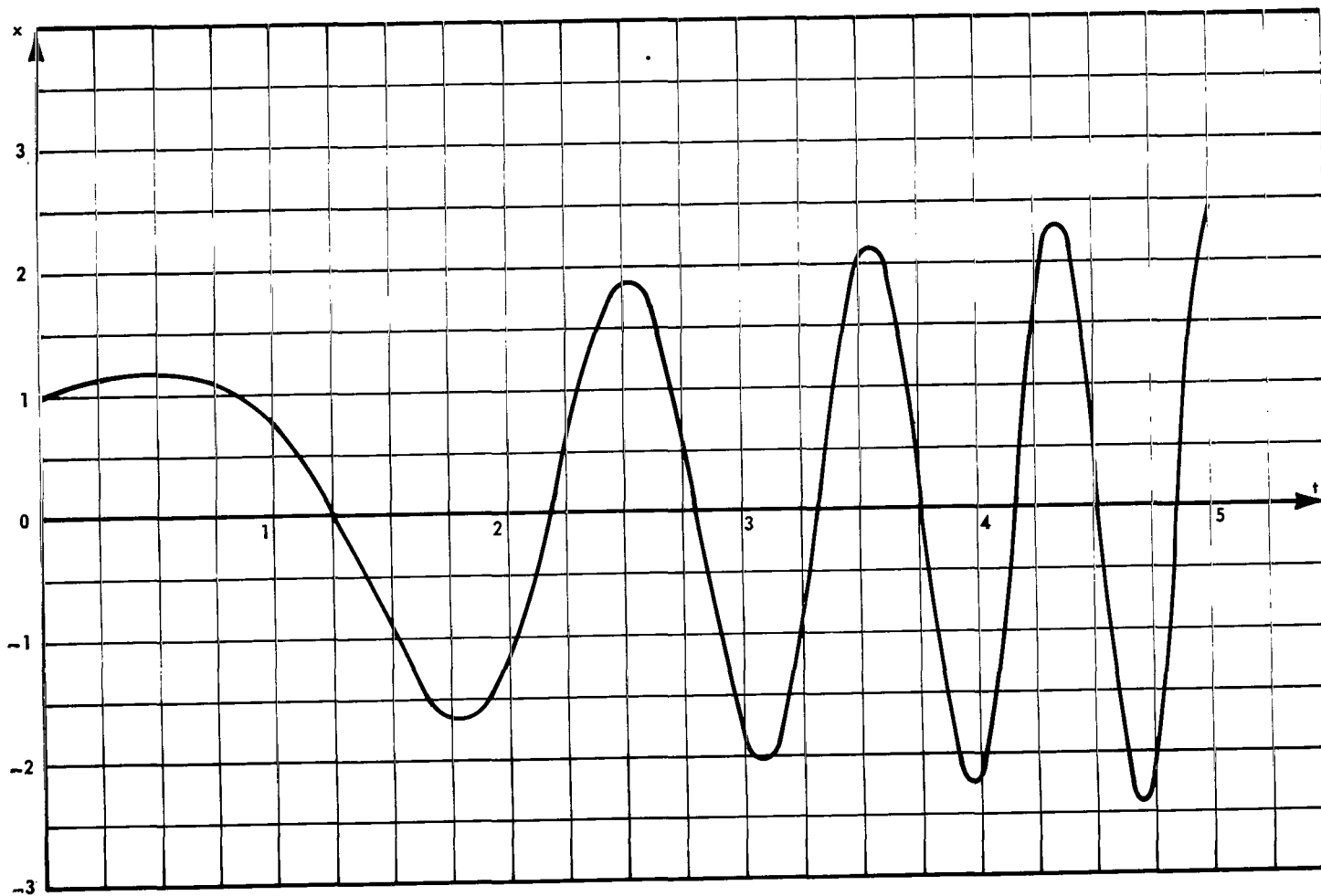


Figure 3. Solution  $x_T = \sqrt{t+1} \cdot \cos(t^2)$  for Problem I.

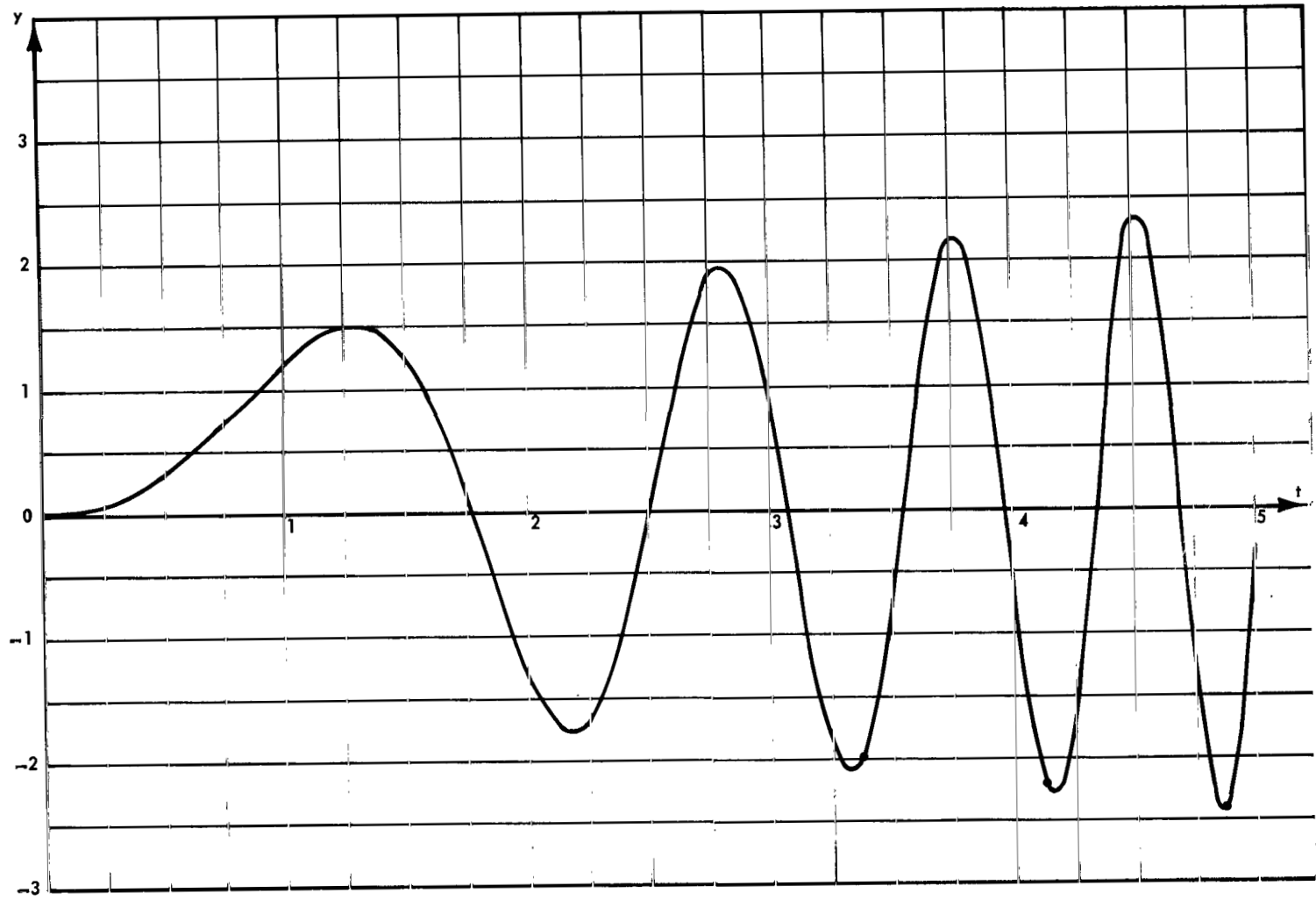


Figure 4. Solution  $y_T = \sqrt{t+1} \cdot \sin(t^2)$  for Problem I.

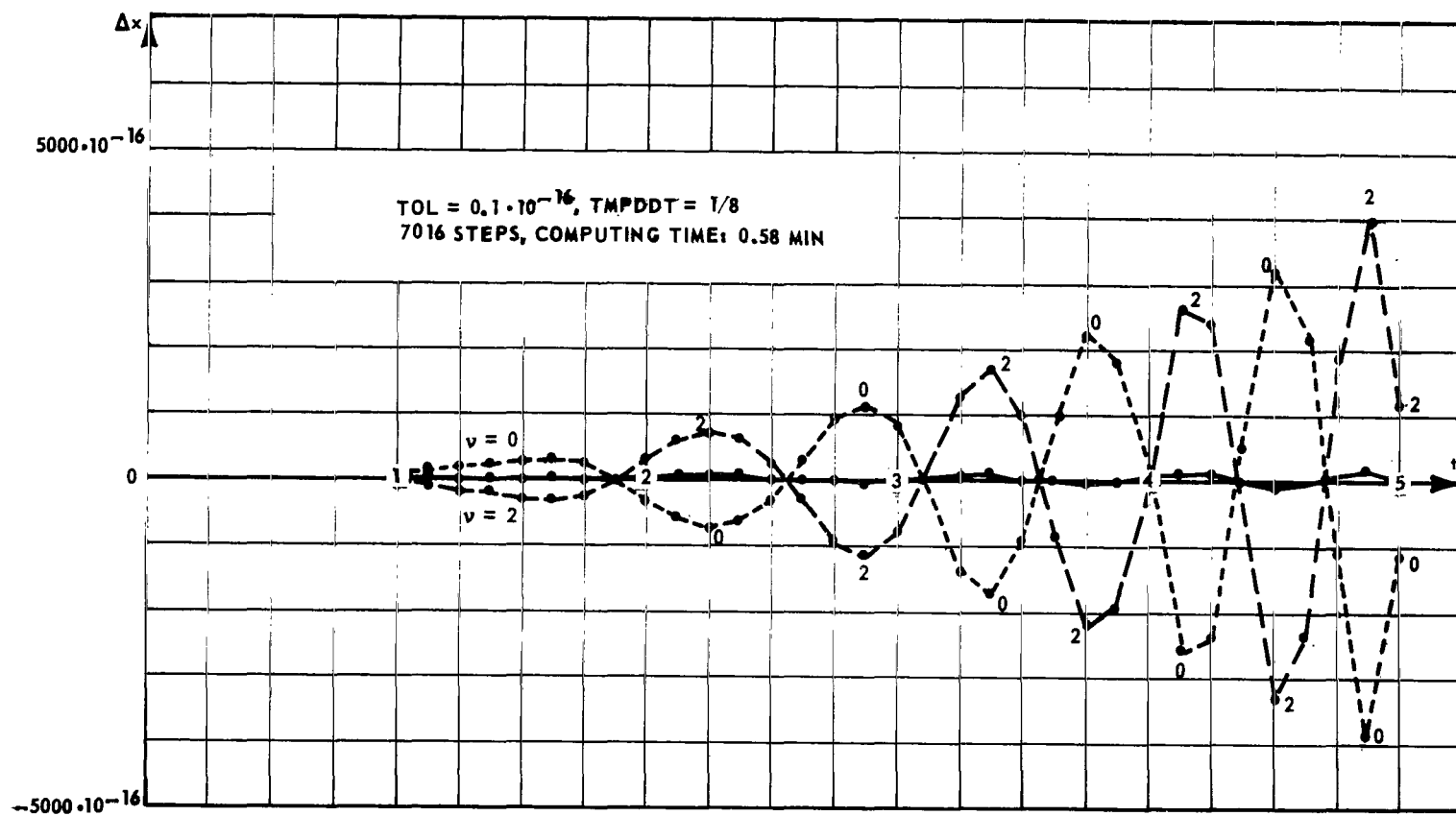


Figure 5. Propagated error  $\Delta x$  for Problem I, using RK5(6) and one integration procedure per step ( $v = 0, 1, 2$ ).

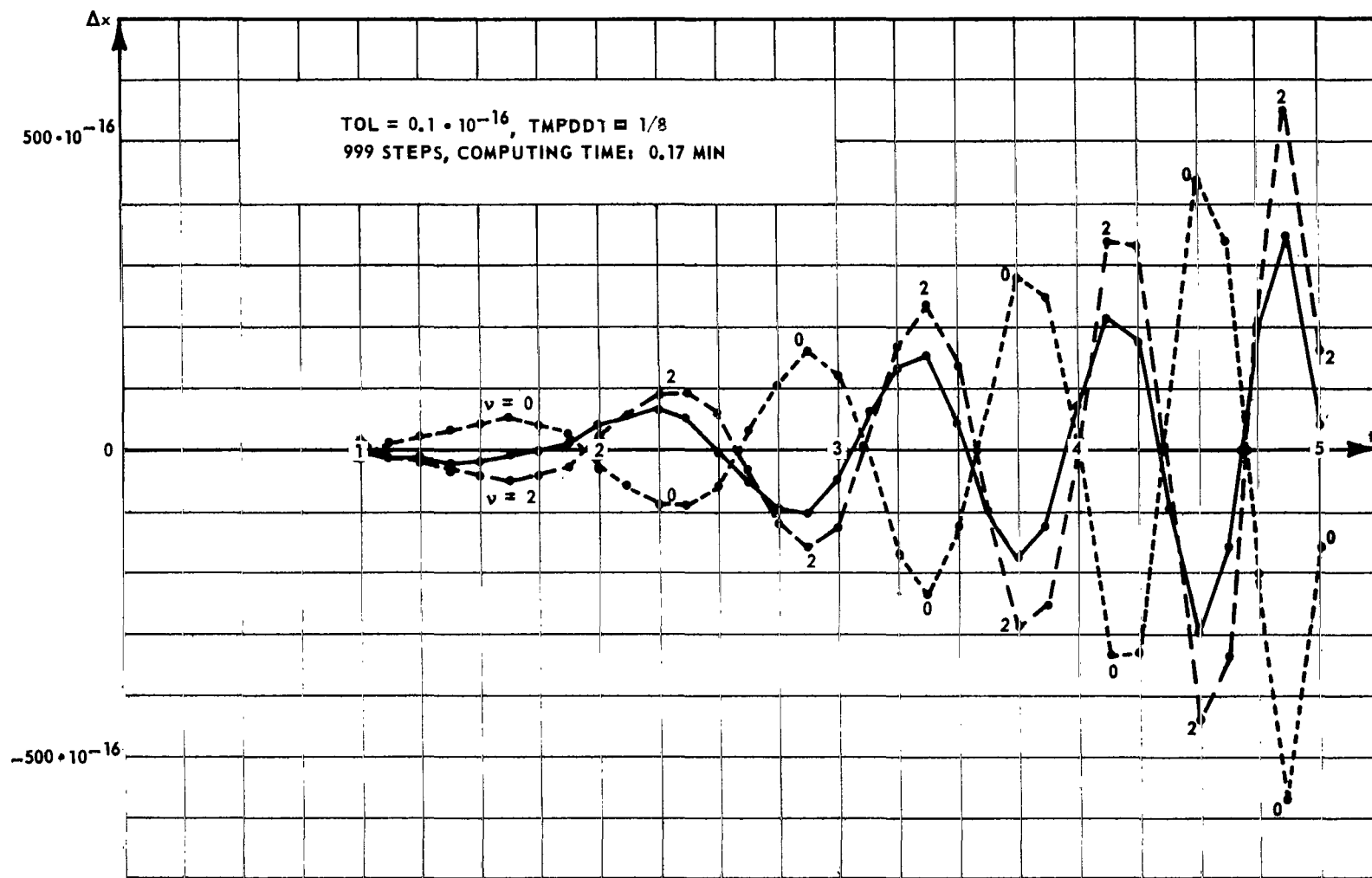
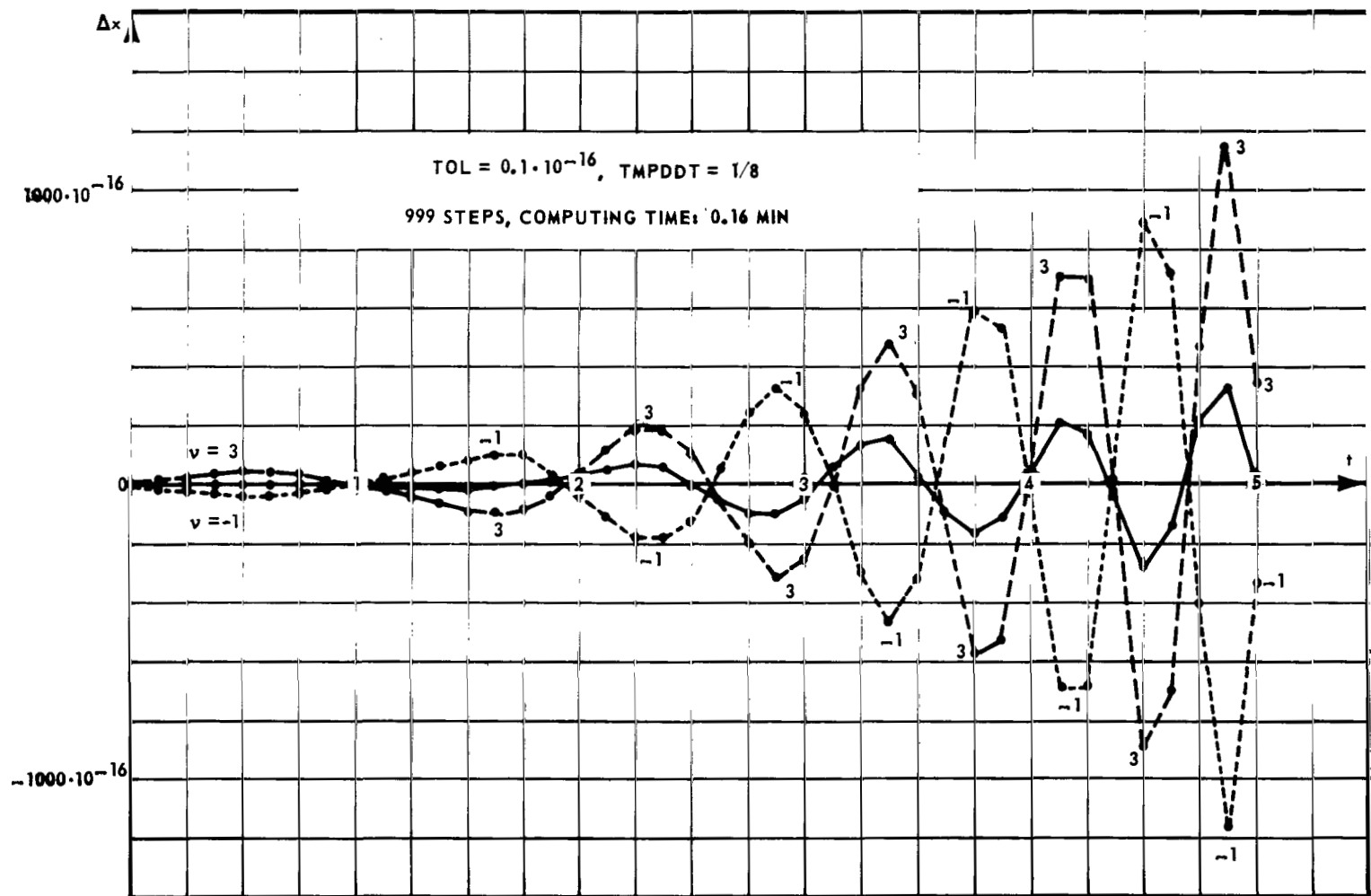


Figure 6. Propagated error  $\Delta x$  for Problem I, using RK7(8) and one integration procedure per step ( $\nu = 0, 1, 2$ ).



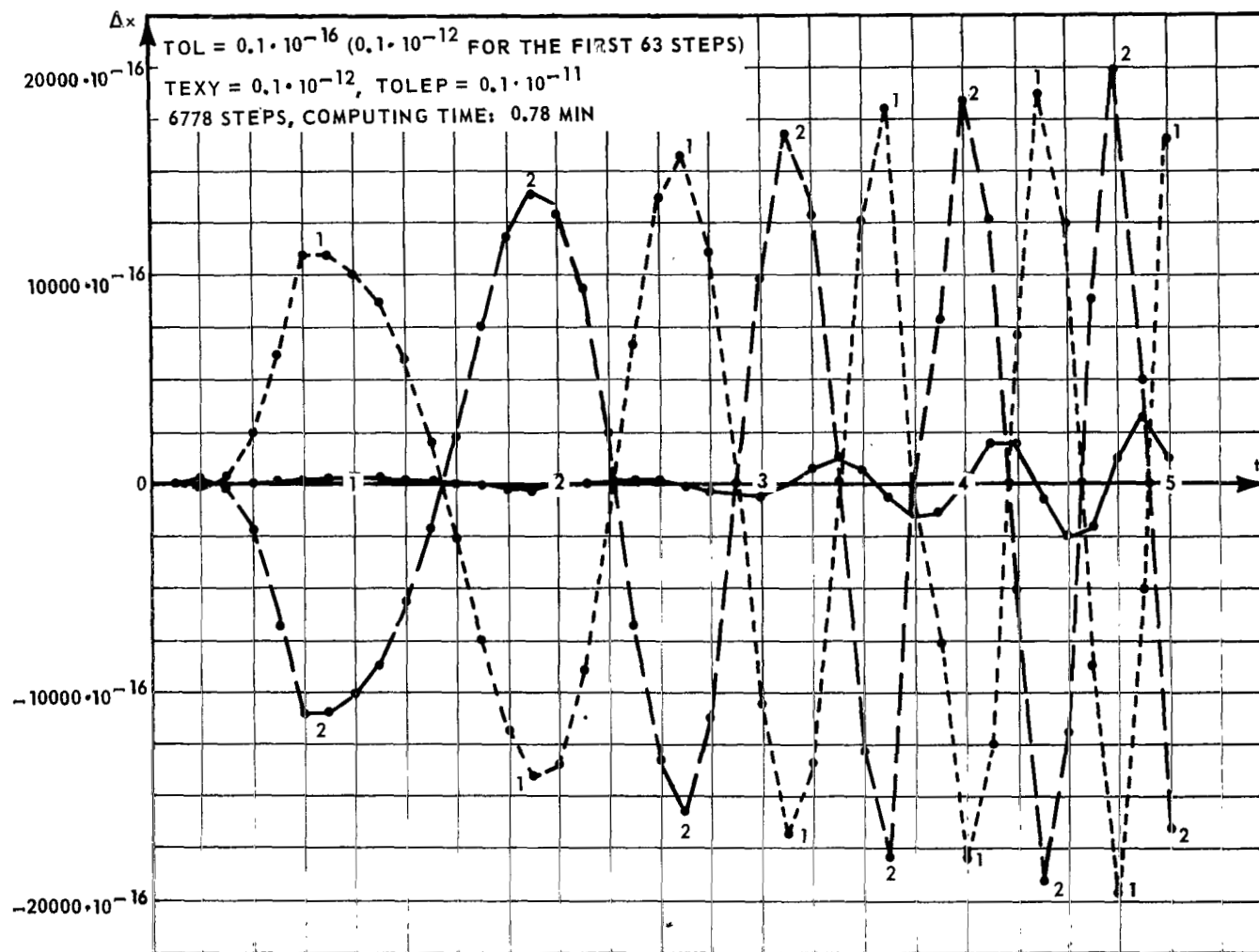


Figure 8. Propagated error  $\Delta x$  for Problem I, using RK5(6) and two integration procedures per step.

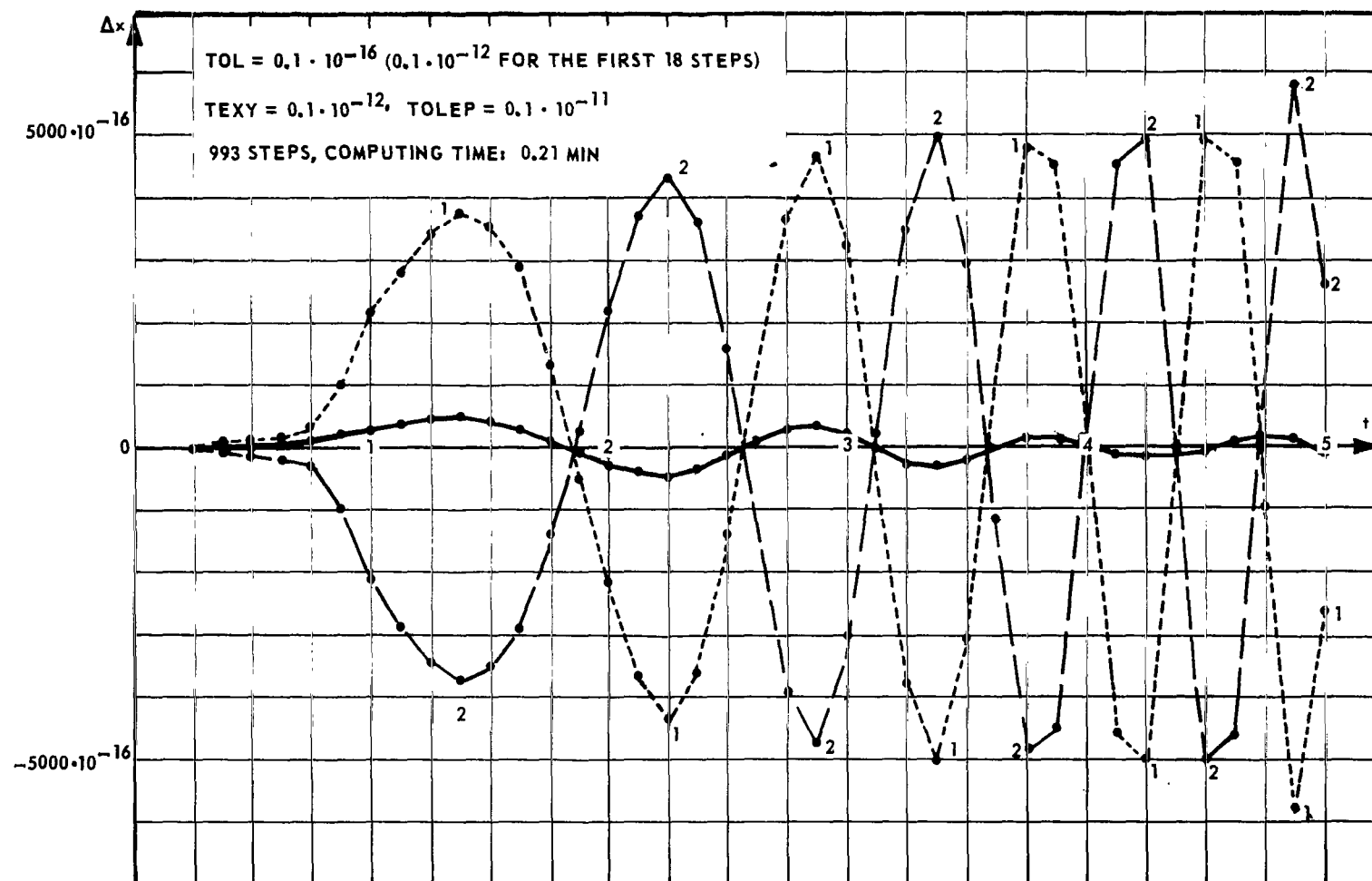


Figure 9. Propagated error  $\Delta x$  for Problem I, using RK7(8) and two integration procedures per step.

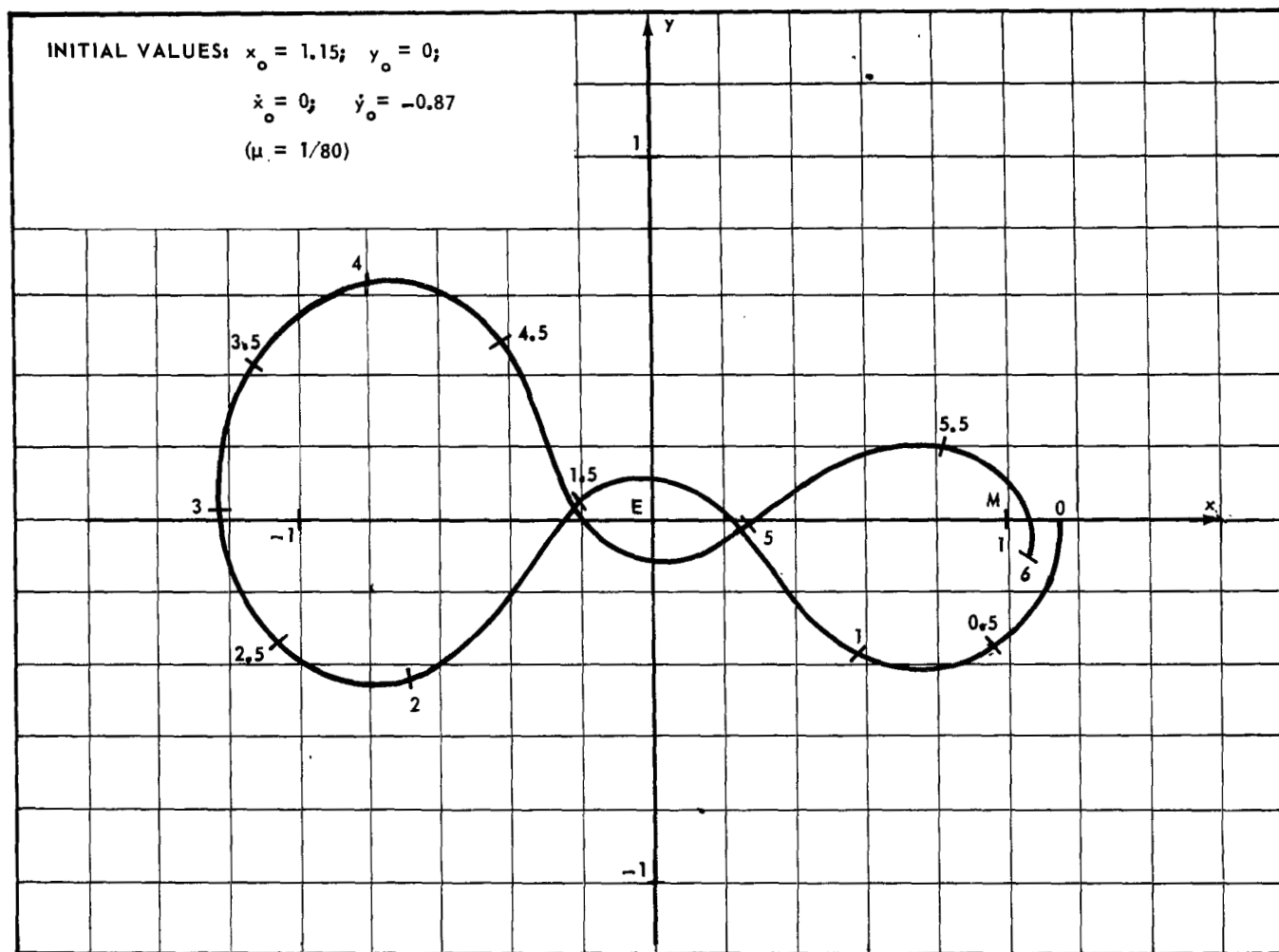


Figure 10. Restricted problem of three bodies: orbit for Problem IIa.



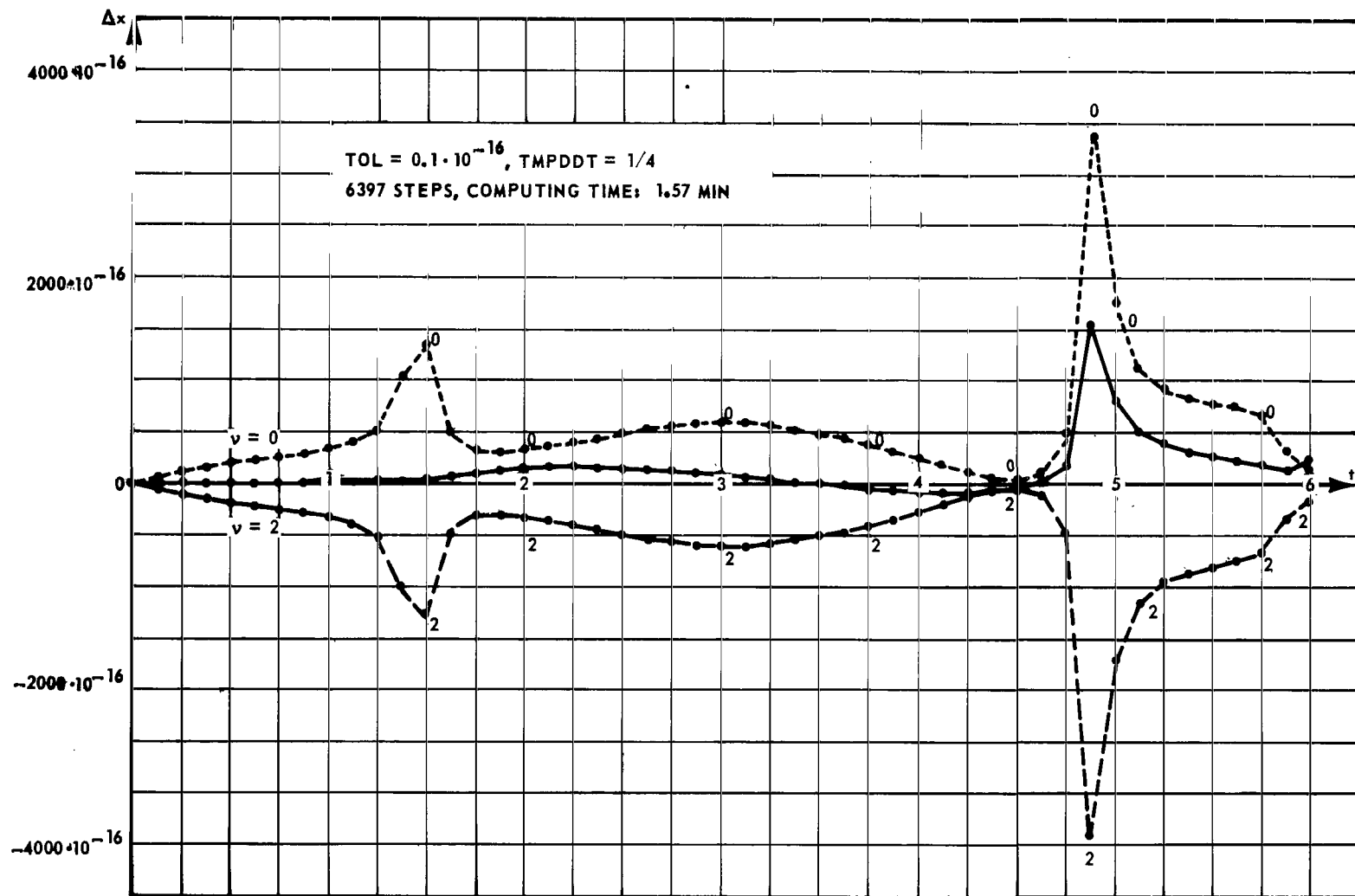


Figure 11. Propagated error  $\Delta x$  for Problem IIa, using RK5(6) and one integration procedure per step ( $\nu = 0, 1, 2$ ).

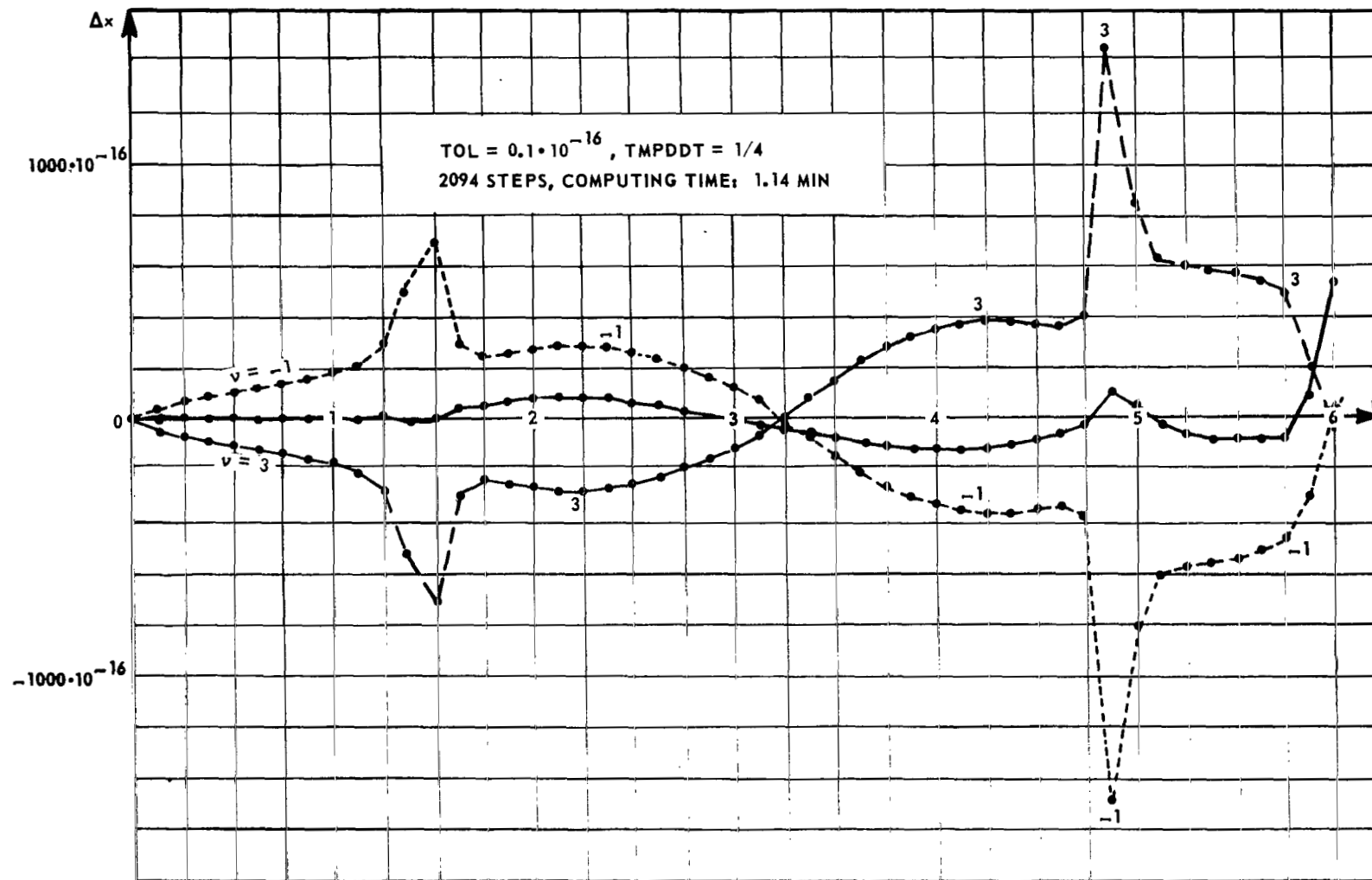


Figure 12. Propagated error  $\Delta x$  for Problem IIa, using RK7(8) and one integration procedure per step ( $\nu = -1, 1, 3$ ).

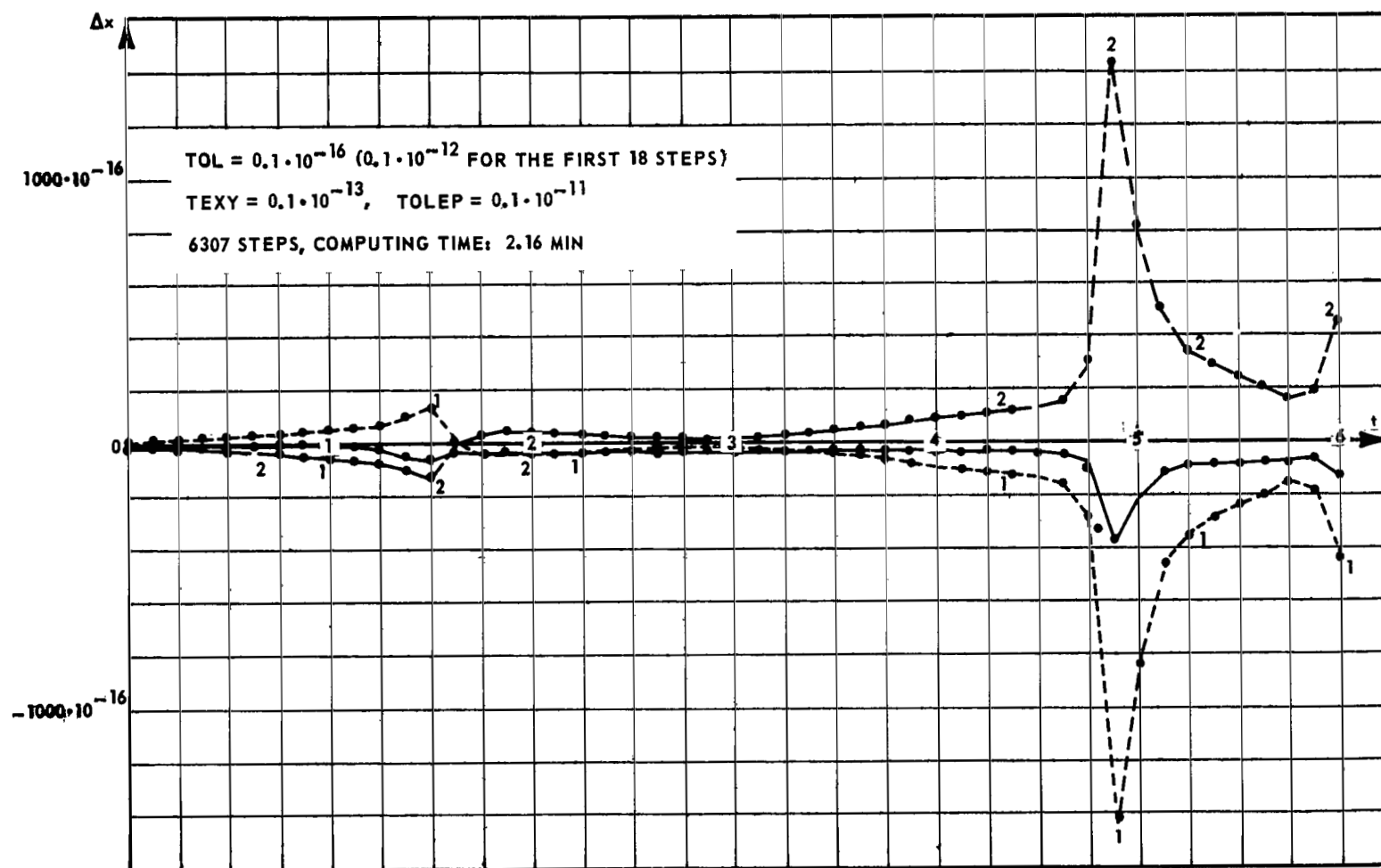


Figure 13. Propagated error  $\Delta x$  for Problem IIa, using RK5(6) and two integration procedures per step.

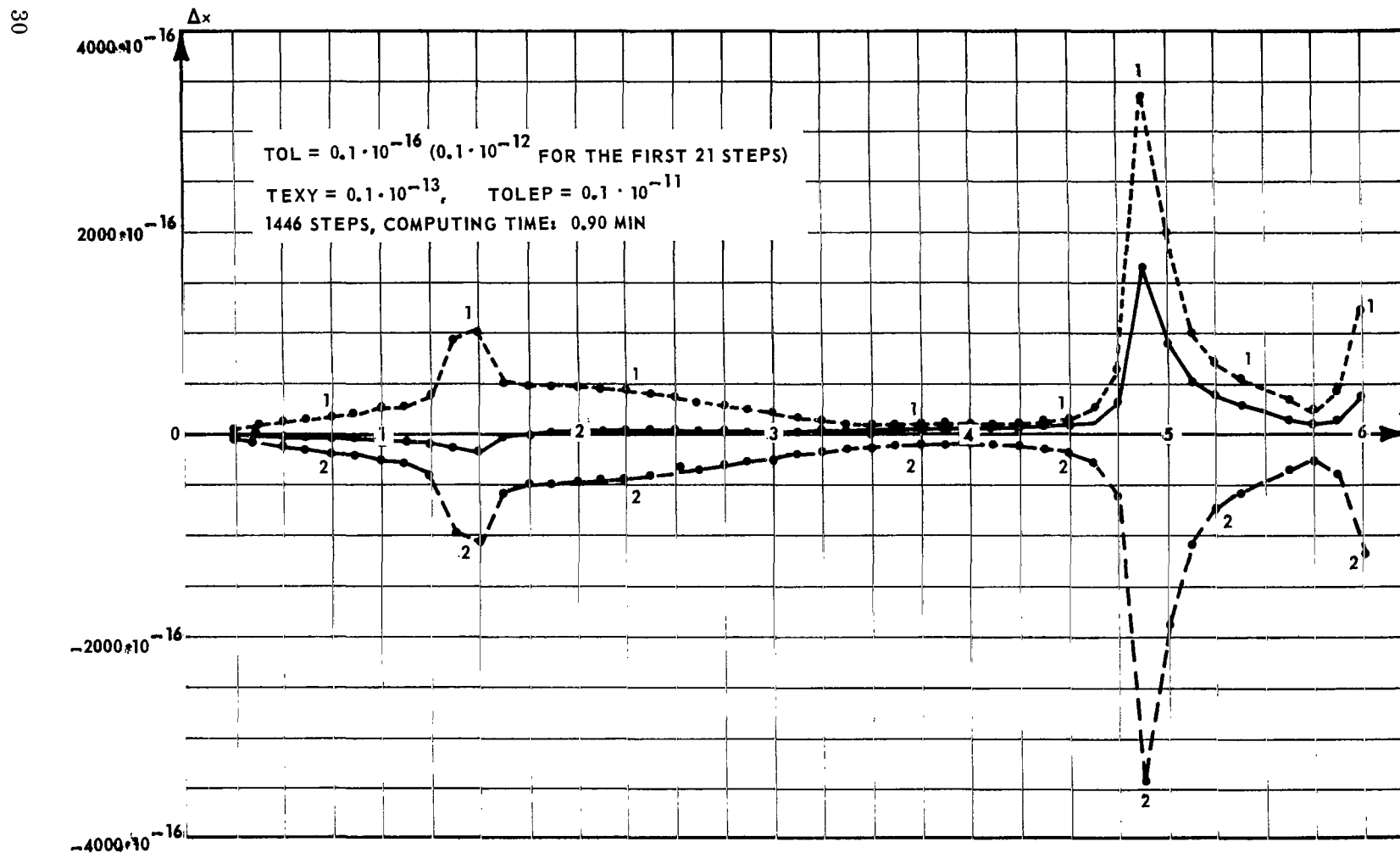


Figure 14. Propagated error  $\Delta x$  for Problem IIa, using RK7(8) and two integration procedures per step.

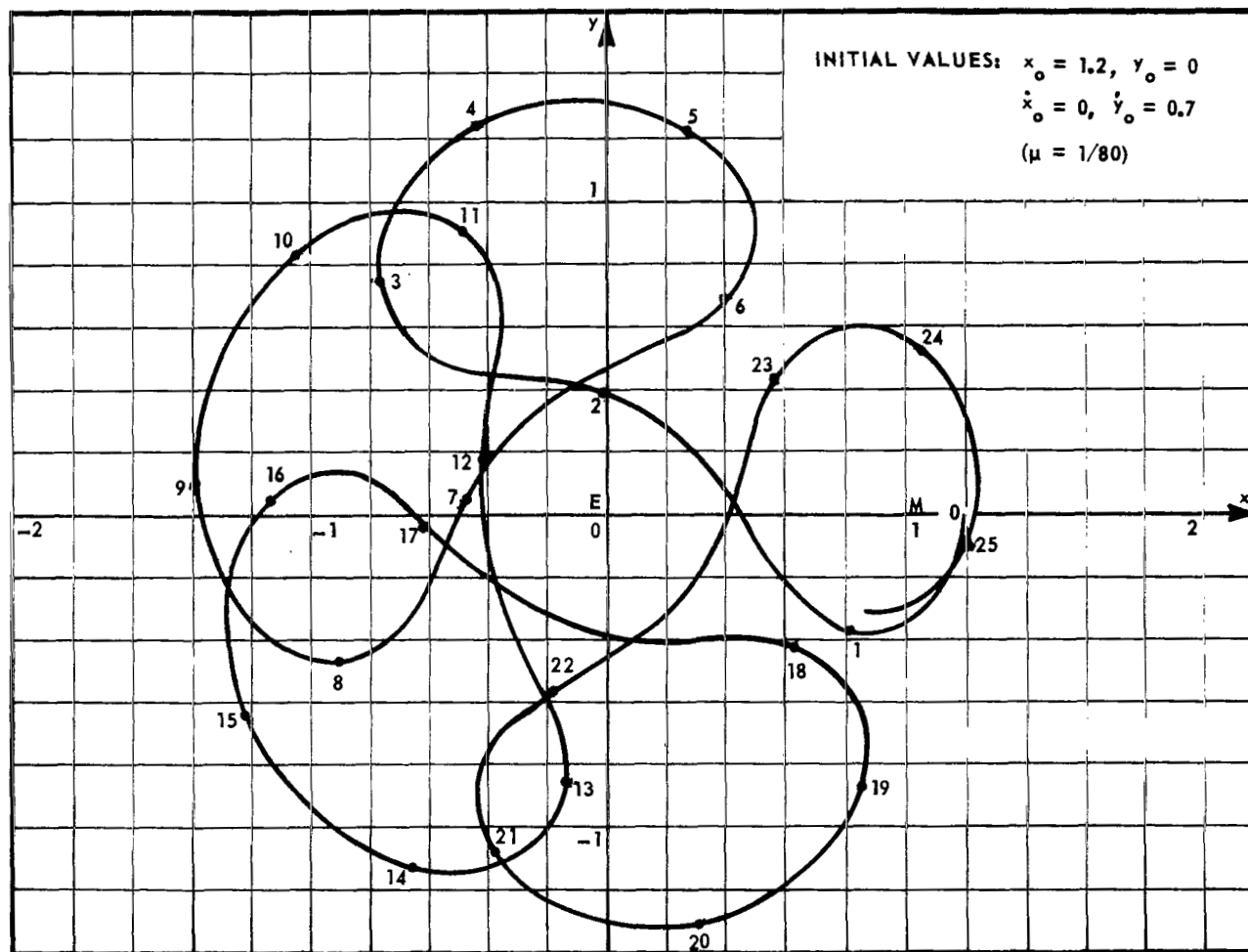


Figure 15. Restricted problem of three bodies: orbit for Problem IIb.

Figure 16. Propagated error  $\Delta x$  for Problem IIb, using RK7(8) and one integration procedure per step ( $\nu = -1, 1, 3$ ).

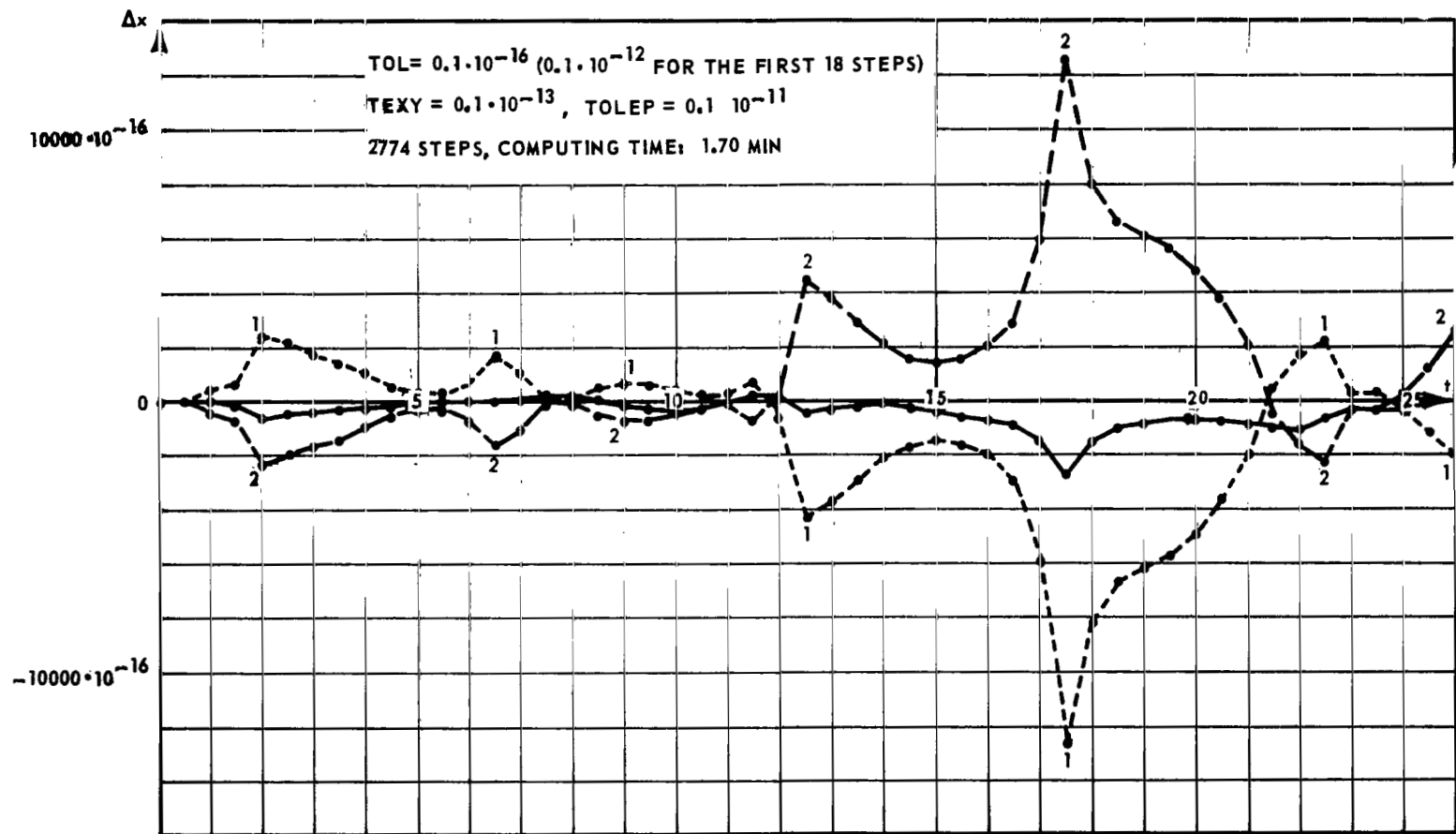


Figure 17. Propagated error  $\Delta x$  for Problem IIb, using RK7(8) and two integration procedures per step.

## APPENDIX

### COEFFICIENTS FOR RUNGE-KUTTA FORMULAS RK1(2), RK2(3), . . . , RK7(8)

RK1(2)

$\begin{array}{c} \lambda \\ \backslash \\ \kappa \end{array}$	$\alpha_{\kappa}$	$\beta_{\kappa\lambda}$		$c_{\kappa}$	$\hat{c}_{\kappa}$
		0	1		
0	0	0		$\frac{1}{8}$	$\frac{1}{16}$
1	$\frac{1}{2}$	$\frac{1}{2}$		$\frac{7}{8}$	$\frac{7}{8}$
2	1	$\frac{1}{8}$	$\frac{7}{8}$		$\frac{1}{16}$

$$TE = \frac{1}{16} (f_0 - f_2) h$$

RK2(3)

$\begin{array}{c} \lambda \\ \backslash \\ \kappa \end{array}$	$\alpha_{\kappa}$	$\beta_{\kappa\lambda}$			$c_{\kappa}$	$\hat{c}_{\kappa}$
		0	1	2		
0	0	0			$\frac{5}{18}$	$\frac{5}{18}$
1	$\frac{1}{2}$	$\frac{1}{2}$			$\frac{1}{6}$	0
2	$\frac{3}{4}$	$\frac{3}{16}$	$\frac{9}{16}$		$\frac{5}{9}$	$\frac{8}{9}$
3	1	$\frac{5}{18}$	$\frac{1}{6}$	$\frac{5}{9}$		$-\frac{1}{6}$

$$TE = \frac{1}{6} (f_1 - 2f_2 + f_3) h$$



# RK3(4)

$\lambda \backslash \kappa$	$\alpha_{\kappa}$	$\beta_{\kappa\lambda}$				$c_{\kappa}$	$\hat{c}_{\kappa}$
		0	1	2	3		
0	0	0				$\frac{79}{490}$	$\frac{229}{1470}$
1	$\frac{2}{7}$	$\frac{2}{7}$				0	0
2	$\frac{7}{15}$	$\frac{77}{900}$	$\frac{343}{900}$			$\frac{2175}{3626}$	$\frac{1125}{1813}$
3	$\frac{35}{38}$	$\frac{805}{1444}$	$-\frac{77175}{54872}$	$\frac{97125}{54872}$		$\frac{2166}{9065}$	$\frac{13718}{81585}$
4	1	$\frac{79}{490}$	0	$\frac{2175}{3626}$	$\frac{2166}{9065}$		$\frac{1}{18}$

$$TE = \left( \frac{4}{735} f_0 - \frac{75}{3626} f_2 + \frac{5776}{81\,585} f_3 - \frac{1}{18} f_4 \right) h$$

# RK4(5)

$\begin{matrix} \backslash \\ \kappa \end{matrix} \lambda$	$\alpha_{\kappa}$	$\beta_{\kappa\lambda}$					$c_{\kappa}$	$\hat{c}_{\kappa}$
		0	1	2	3	4		
0	0	0					$\frac{25}{216}$	$\frac{16}{135}$
1	$\frac{1}{4}$	$\frac{1}{4}$					0	0
2	$\frac{3}{8}$	$\frac{3}{32}$	$\frac{9}{32}$				$\frac{1408}{2565}$	$\frac{6656}{12825}$
3	$\frac{12}{13}$	$\frac{1932}{2197}$	$-\frac{7200}{2197}$	$\frac{7296}{2197}$			$\frac{2197}{4104}$	$\frac{28561}{56430}$
4	1	$\frac{439}{216}$	-8	$\frac{3680}{513}$	$-\frac{845}{4104}$		$-\frac{1}{5}$	$-\frac{9}{50}$
5	$\frac{1}{2}$	$-\frac{8}{27}$	2	$-\frac{3544}{2565}$	$\frac{1859}{4104}$	$-\frac{11}{40}$		$\frac{2}{55}$

$$TE = \left( -\frac{1}{360} f_0 + \frac{128}{4275} f_2 + \frac{2197}{75 \cdot 240} f_3 - \frac{1}{50} f_4 - \frac{2}{55} f_5 \right) h$$

RK5(6)

$\kappa \backslash \lambda$	$\alpha_{\kappa}$	$\beta_{\kappa\lambda}$								$c_{\kappa}$	$\hat{c}_{\kappa}$
		0	1	2	3	4	5	6			
0	0	0							$\frac{31}{384}$	$\frac{7}{1408}$	
1	$\frac{1}{6}$	$\frac{1}{6}$							0		
2	$\frac{4}{15}$	$\frac{4}{75}$	$\frac{16}{75}$						$\frac{1125}{2816}$		
3	$\frac{2}{3}$	$\frac{5}{6}$	$-\frac{8}{3}$	$\frac{5}{2}$					$\frac{9}{32}$		
4	$\frac{4}{5}$	$-\frac{8}{5}$	$\frac{144}{25}$	-4	$\frac{16}{25}$				$\frac{125}{768}$		
5	1	$\frac{361}{320}$	$-\frac{18}{5}$	$\frac{407}{128}$	$-\frac{11}{80}$	$\frac{55}{128}$			$\frac{5}{66}$	0	
6	0	$-\frac{11}{640}$	0	$\frac{11}{256}$	$-\frac{11}{160}$	$\frac{11}{256}$	0			$\frac{5}{66}$	
7	1	$\frac{93}{640}$	$-\frac{18}{5}$	$\frac{803}{256}$	$-\frac{11}{160}$	$\frac{99}{256}$	0	1		$\frac{5}{66}$	

$$TE = \frac{5}{66} (f_0 + f_5 - f_6 - f_7) h$$

RK6(7)

$\kappa \backslash \lambda$	$\alpha_{\kappa}$	$\beta_{\kappa\lambda}$								$c_{\kappa}$	$\hat{c}_{\kappa}$
		0	1	2	3	4	5	6	7		
0	0	0								$\frac{77}{1440}$	$\frac{11}{864}$
1	$\frac{2}{33}$	$\frac{2}{33}$								0	
2	$\frac{4}{33}$	0	$\frac{4}{33}$							0	
3	$\frac{2}{11}$	$\frac{1}{22}$	0	$\frac{3}{22}$						$\frac{1771561}{6289920}$	
4	$\frac{1}{2}$	$\frac{43}{64}$	0	$-\frac{165}{64}$	$\frac{77}{32}$					$\frac{32}{105}$	
5	$\frac{2}{3}$	$-\frac{2383}{486}$	0	$\frac{1067}{54}$	$-\frac{26312}{1701}$	$\frac{2176}{1701}$				$\frac{243}{2560}$	
6	$\frac{6}{7}$	$\frac{10077}{4802}$	0	$-\frac{5643}{686}$	$\frac{116259}{16807}$	$-\frac{6240}{16807}$	$\frac{1053}{2401}$			$\frac{16807}{74880}$	
7	1	$-\frac{733}{176}$	0	$\frac{141}{8}$	$-\frac{335763}{23296}$	$\frac{216}{77}$	$-\frac{4617}{2816}$	$\frac{7203}{9152}$		$\frac{11}{270}$	0
8	0	$\frac{15}{352}$	0	0	$-\frac{5445}{46592}$	$\frac{18}{77}$	$-\frac{1215}{5632}$	$\frac{1029}{18304}$	0		$\frac{11}{270}$
9	1	$-\frac{1833}{352}$	0	$\frac{141}{8}$	$-\frac{51237}{3584}$	$\frac{18}{7}$	$-\frac{729}{512}$	$\frac{1029}{1408}$	0	1	$\frac{11}{270}$

$$TE = \frac{11}{270} (f_0 + f_7 - f_8 - f_9) h$$

RK7(8)

$\kappa \backslash \lambda$	$\alpha_{\kappa}$	$\beta_{\kappa\lambda}$											$c_{\kappa}$	$\hat{c}_{\kappa}$
		0	1	2	3	4	5	6	7	8	9	10	11	
0	0	0												$\frac{41}{840}$   0
1	$\frac{2}{27}$	$\frac{2}{27}$												0
2	$\frac{1}{9}$	$\frac{1}{36}$	$\frac{1}{12}$											0
3	$\frac{1}{6}$	$\frac{1}{24}$	0	$\frac{1}{8}$										0
4	$\frac{5}{12}$	$\frac{5}{12}$	0	$-\frac{25}{16}$	$\frac{25}{16}$									0
5	$\frac{1}{2}$	$\frac{1}{20}$	0	0	$\frac{1}{4}$	$\frac{1}{5}$								$\frac{34}{105}$
6	$\frac{5}{6}$	$-\frac{25}{108}$	0	0	$\frac{125}{108}$	$-\frac{65}{27}$	$\frac{125}{54}$							$\frac{9}{35}$
7	$\frac{1}{6}$	$\frac{31}{300}$	0	0	0	$\frac{61}{225}$	$-\frac{2}{9}$	$\frac{13}{900}$						$\frac{9}{35}$
8	$\frac{2}{3}$	2	0	0	$-\frac{53}{6}$	$\frac{704}{45}$	$-\frac{107}{9}$	$\frac{67}{90}$	3					$\frac{9}{280}$
9	$\frac{1}{3}$	$-\frac{91}{108}$	0	0	$\frac{23}{108}$	$-\frac{976}{135}$	$\frac{311}{54}$	$-\frac{19}{60}$	$\frac{17}{6}$	$-\frac{1}{12}$				$\frac{9}{280}$
10	1	$\frac{2383}{4100}$	0	0	$-\frac{341}{164}$	$\frac{4496}{1025}$	$-\frac{301}{82}$	$\frac{2133}{4100}$	$\frac{45}{82}$	$\frac{45}{164}$	$\frac{18}{41}$			$\frac{41}{840}$   0
11	0	$\frac{3}{205}$	0	0	0	0	$-\frac{6}{41}$	$-\frac{3}{205}$	$-\frac{3}{41}$	$\frac{3}{41}$	$\frac{6}{41}$	0		$\frac{41}{840}$
12	1	$-\frac{1777}{4100}$	0	0	$-\frac{341}{164}$	$\frac{4496}{1025}$	$-\frac{289}{82}$	$\frac{2193}{4100}$	$\frac{51}{82}$	$\frac{33}{164}$	$\frac{12}{41}$	0	1	$\frac{41}{840}$

$$TE = \frac{41}{840} (f_0 + f_{10} - f_{11} - f_{12})h$$

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